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Lattice models provide fast and accurate way to simulate DNA self-assembling FREE

Adam Liebendorfer

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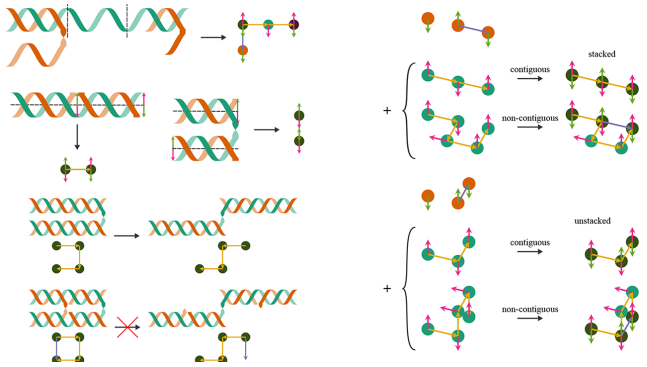
Lattice modeling coupled with Monte Carlo methods allows accurate and logistically feasible computational simulations of DNA folding.



It has been known for decades that DNA can function as a versatile design material for building nanostructures. One technique, known as the DNA origami method, uses shorter "staple" strands to fold a longer single strand of DNA and manipulate into a target shape. While DNA nanostructure design has become increasingly complex, few models exist that provide accurate simulations of DNA self-assembly in a computationally feasible way.

Cumberworth et al. proposed a model using Monte Carlo methods that balances the need for accuracy within the confines of current computing power. The model represents DNA origami on a lattice, yet retains information about the helicity of double-stranded DNA and the strength of DNA hybridization. By using a combination of computational techniques such as grand canonical simulations, replica exchange Monte Carlo and movements originally designed for polymer lattice models, Cumberworth et al. improved the efficiency of sampling the configuration space. This is important as the ability to obtain good sampling of assembled states in a short period of time opens up the possibility of studying DNA origami designs more systematically.

Their representation of a helix phase, along with the rules they chose to apply to the representation in order to capture the helical twist constraints, are "perhaps the most innovative part of our model," according to Alexander Cumberworth, an author on the paper.

Looking ahead, the authors plan to use their model to look at which factors might be used to provide finer control over the thermodynamic stability of assembled states. Additionally, they hope to examine kinetic barriers to self-assembly, and study how changes to design conditions can be used to optimize assembly kinetics.

They intend to make a user-friendly version of their software freely available.

Source: "Lattice models and Monte Carlo methods for simulating DNA origami self-assembly," by Alexander Cumberworth, Aleks Reinhardt, and Daan Frenkel, *The Journal of Chemical Physics* (2018). The article can be accessed at https://doi.org/10.1063/1.5051835.